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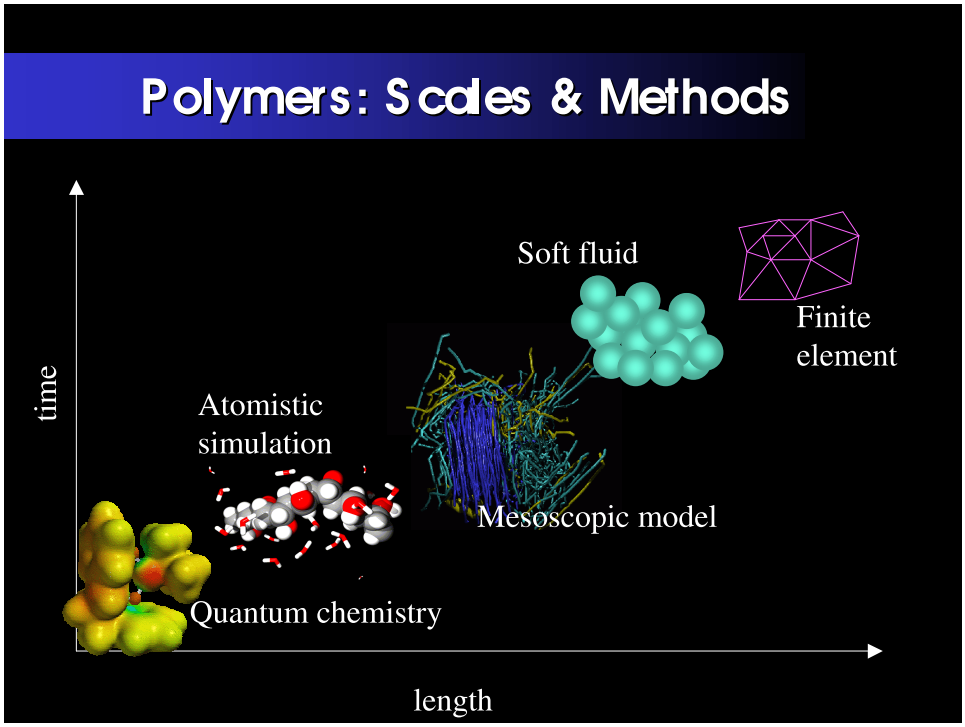
In our daily life we are inevitably constantly confronted with the properties of polymer materials, or more general "soft matter materials". On the one hand we ourselves largely consist of soft matter (bio polymers, such as DNA, proteins, and lipids which form the cell membranes ...) plus some minerals and a lot of water and, on the other hand, our daily life is not longer conceivable without goods containing polymers. The technical and commercial applications range from rather simple commodity polymer products ("plastics") such as polyethylene for plastic bags through polymers for high tech applications such as polycarbonate for CDs or DVDs, all the way to electronic applications (laser materials, circuit boards for the semiconductor industry). While most synthetic polymers are not water soluble, some and most bio polymers certainly are water soluble. Such systems find widespread application in the environment and hygiene sector (water treatment, super absorbers) or as food additives and/or pharmaceutical products, not to speak of the natural abundance and relevance for all living organisms (e. g. cellulose). This demonstrates the relevance of "soft matter" and with no doubt gives rise to intense technological investigations.

However, why are such systems of scientific interest? Above all applications polymers are intriguing molecules by themselves which pose many intellectual challenges in their own right. The fact that many such problems are close to biological questions and/or technical problems just adds another momentum. The characteristic feature of soft matter is their molecular structure. Unlike conventional solids or liquids, polymers are extended molecules (e. g. long chain molecules), where the overall diameter easily reaches hundreds of times of that of a typical small molecule such as water. The properties are governed by a combination of interaction energy (local submolecule-submolecule interaction) and entropy resulting from the many possible conformations such a huge molecule can obtain. Consequently, deformations of a polymer system typically only weakly change the energies but significantly the entropy per chain. Since the chains are huge, the effective particle density (polymer density) is small allowing for a relatively weak response: the systems are, compared to conventional solids, "soft". The typical energy scale is of the order of the thermal energy k_BT. This makes them unique in many respects, but also difficult to understand with conventional, though very advanced, paper and pencil theory. Therefore, already for many years attempts have been undertaken to employ computer simulations in order to study soft matter. First, dating back to the '50s of last century, polymer chains were modeled by self repelling paths on lattices. This approach can be viewed to be of a similar importance to polymer simulations as the Ising model turned out to be for magnetism. However, as the examples of this volume show, meanwhile one goes very much beyond that approach. The different approaches employed nowadays are illustrated in the figure (courtesy F. Müller-Plathe).



The present contributions concentrate on the mesoscopic model regime. They span from test cases for finite size effects in phase transitions via morphology development and dynamics in melts and mixtures, polyelectrolytes in bulk solution and near surfaces to properties of membranes close to applications in biophysics:

Due to the extended size of the whole molecules each chain encounters the presence of many other chains, the effective interaction becomes a long range interaction. Such systems display mean field properties up to a regime very close to the critical point, where the range of the correlation functions, which diverge at the critical point, clearly exceeds the size of the chains. This crossover from meanfield to the Ising critical behaviour is the main subject of the contribution by Binder, Luijten, Houdayer and Müller. In another contribution by Binder, Baschnagel and Müller chain dynamics as well as collective dynamics of melts far away and in proximity to the glass transition is studied. This also includes the phase separation kinetics and morphology developments of mixtures in bulk and especially thin films.

A second group of two papers deals with polyelectrolytes in solution (Holm, Kremer) and polyelectrolyte brushes (Seidel). Most polyelectrolytes are only water soluble due to the dissociation of small ions. The typical hydrocarbon backbone is highly hydrophobic. This leads to a competition of the ion induced solubility of the chains and an effectively attractive interaction of the chain beads. The consequences of this competition are subject of the first contribution. There, also another topic is addressed. If the electrostatic interaction becomes strong enough, an overall neutral system tries to collapse, for polyelectrolytes this means they are falling out of solution. For semi-flexible systems that leads to aggregation

phenomena, as e. g. found in DNA. This is the second topic of that paper. Ch. Seidel in his contribution addresses a similar problem however for polyelectrolyte brushes. He studies as a function of grafting density, chain length and charge density the chain conformation and determines a structure diagram.

A rather different class of systems is studied by Shillock and Lipowsky. They determine by a rather novel approach, namely dissipative particle dynamics (DPD) properties of liquid model membranes, as they are the prime constituents of biological membranes. This new method allows to study much bigger model systems compared to the so far employed standard models.

All these studies require a joint effort on the hardware side, as it is provided through the computer time grants of the NIC, and on the software side. The second is, where all the efforts of the different research groups goes in order to perform competitive simulations. The CPU time needed for the different project varied between about 50000 processor hours per year and 50000 processor hours (T3E) total for the whole project, while the number of used CPU hours on the vector machines of course is much smaller.